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14. ABSTRACT New multiscale methods have been developed for the study of microcracking and dislocations. The multiscale method for microcracking aggregates the effect of an arbitrary number of cracks at the micro level into a single equivalent crack at the macrolevel. The methodology is based on the concept of a perforated unit cell, which excludes all subdomains of the unit cell where the material loses stability in the averaging operations. We have shown that for this approach, the macro bulk material does not lose ellipticity when failure occurs. This is an				
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## Abstract

New multiscale methods have been developed for the study of microcracking and dislocations. The multiscale method for microcracking aggregates the effect of an arbitrary number of cracks at the micro level into a single equivalent crack at the macrolevel. The methodology is based on the concept of a perforated unit cell, which excludes all subdomains of the unit cell where the material loses stability in the averaging operations. We have shown that for this approach, the macro bulk material does not lose ellipticity when failure occurs. This is an important development since it avoids the ill-posedness usually associated with multiscale modeling of failure. Comparisons with direct numerical simulations show excellent accuracy. We have also developed new models for dislocations and concurrent methods that couple atomistic models with these new continuum dislocation methods. These enable dislocation dynamics in arbitrary geometries and materials to be modeled in terms of fundamental physics.

## Statement of the Problem Studied

Two problems were studied in this investigation:

1. the multiscale modeling of failure
2. the multiscale modeling of dislocations

The multiscale modeling of failure remains an unresolved problem because when a subscale model predicts that the stress-strain behavior at the coarser scale loses ellipticity, the coarse scale model becomes ill-posed. Consequently, the results of the coarse-scale model become very mesh dependent and unreliable. This occurs for example when microcracking takes place at the finer scale. The objective of this investigation was to develop methods for circumventing these difficulties by separating out the unstable material behavior at the finer scale into an equivalent discontinuity and traction. The failure behavior at the fine scale is thus isolated as either a crack, shear band or dislocation at the coarser scale. This is in agreement with observed physics of failure processes, since they are always associated with the aforementioned phenomena.

Dislocations are closely related phenomena which are associated with plasticity. Dislocations are characterized by relative atomic displacements at the crystalline level which can be characterized by discontinuities at the macrolevel. In this work, new methods have been developed for modeling dislocations by the extended finite element method. Furthermore, methods have been developed for coupling continuum models of dislocations with atomistic models. These coupled multiscale models will allow investigators to bypass the heuristic, phenomenological rules which are used to drive the displacements of dislocation cores in dislocation dynamics models.

## Summary of Important Results

It has been found that ill-posedness can be avoided in both hierarchical and semiconcurrent couplings of multiscale models through the use of two key concepts. The first key concept is the definition of a perforated representative volume element (or unit cell) which excludes all material points that are unstable (to be more precise, not convex). The second key concept is a method for defining an equivalent discontinuity in terms of the behavior of the perforated unit cell. The method is called the multiscale aggregating discontinuity method (MAD).

Let the perforated subdomain of the unit cell  $\Omega_0^m$  be denoted by  $\tilde{\Omega}_0^m$ . The macroscale first Piola-Kirchhoff stress  $\mathbf{P}^M$  is then defined in terms of the microscale first Piola-Kirchhoff stress  $\mathbf{P}^m$  by

$$\mathbf{P}^M = \frac{1}{|\tilde{\Omega}_0^m|} \int_{\tilde{\Omega}_0^m} \mathbf{P}^m \, d\Omega_0 \quad (1.1)$$

Similarly the macroscale deformation gradient  $\mathbf{F}^M$  is defined in terms of the microscale deformation gradient  $\mathbf{F}^m$  by

$$\mathbf{F}^M = \frac{1}{|\tilde{\Omega}_0^m|} \int_{\tilde{\Omega}_0^m} \mathbf{F}^m \, d\Omega_0 \quad (1.2)$$

Let the motion  $\phi^m(\mathbf{X}^m, t)$  on the sides of the unit cell be given by

$$\phi^m(\mathbf{X}^m, t) = \mathcal{F}^M \cdot \mathbf{X}^m \quad \text{on } \mathbf{X}^m \in \partial\Omega_0^m \quad (1.3)$$

We have shown that an equivalent discontinuity at the macrolevel  $\mathbf{U}^M$  with normal  $\mathbf{N}^M$  can then be extracted by

$$(\mathbf{U}^M, \mathbf{N}^M) = \arg \left( \min_{\mathbf{U}, \mathbf{N}} \left( \mathbf{U}^M \otimes \mathbf{N}^M - |\tilde{\Omega}_0^m| \left( \langle \mathbf{F}^M \rangle - \mathcal{F}^M \right) \right)^2 \right) \quad (1.4)$$

This macroscale discontinuity is then injected into the macroscale model. The forces required to enforce this discontinuity are the traction across the macrocrack.

We have shown that the macroscale model is elliptic as long if the perforated unit cell excludes all material that is not convex. To put this in more precise terms, recall that the convexity of the micromaterial requires that

$$\mathbf{F}^m : \mathbf{C}^m : \mathbf{F}^m > 0 \quad \forall \mathbf{F}^m \quad (1.5)$$

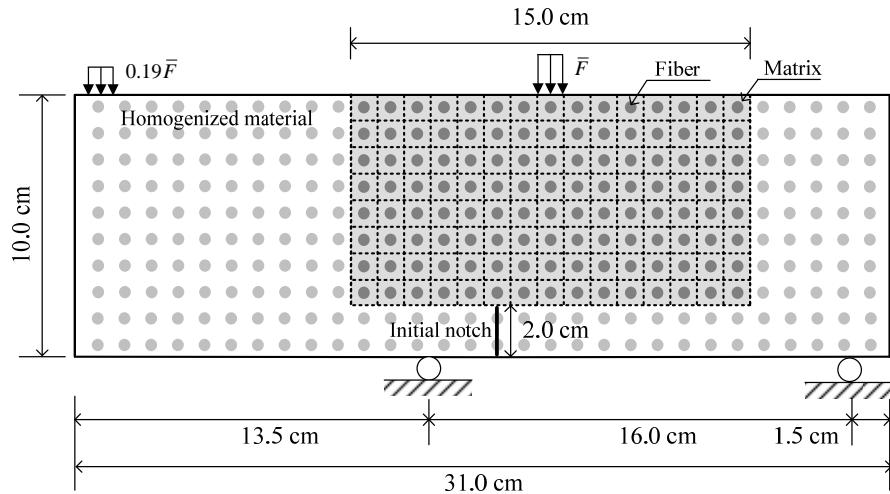
where  $\mathbf{C}^m$  is the tangent modulus for the micromaterial. Ellipticity of the macromaterial requires that

$$\mathbf{g} \otimes \mathbf{h} : \mathbf{C}^M : \mathbf{g} \otimes \mathbf{h} > 0 \quad \forall \mathbf{g} \text{ and } \mathbf{h} \quad (1.6)$$

It has been shown in Belytschko et al. [1] that Equation (1.5) implies (1.6) for the method as described. Therefore the multiscale aggregating equivalent discontinuity method guarantees well-posedness.

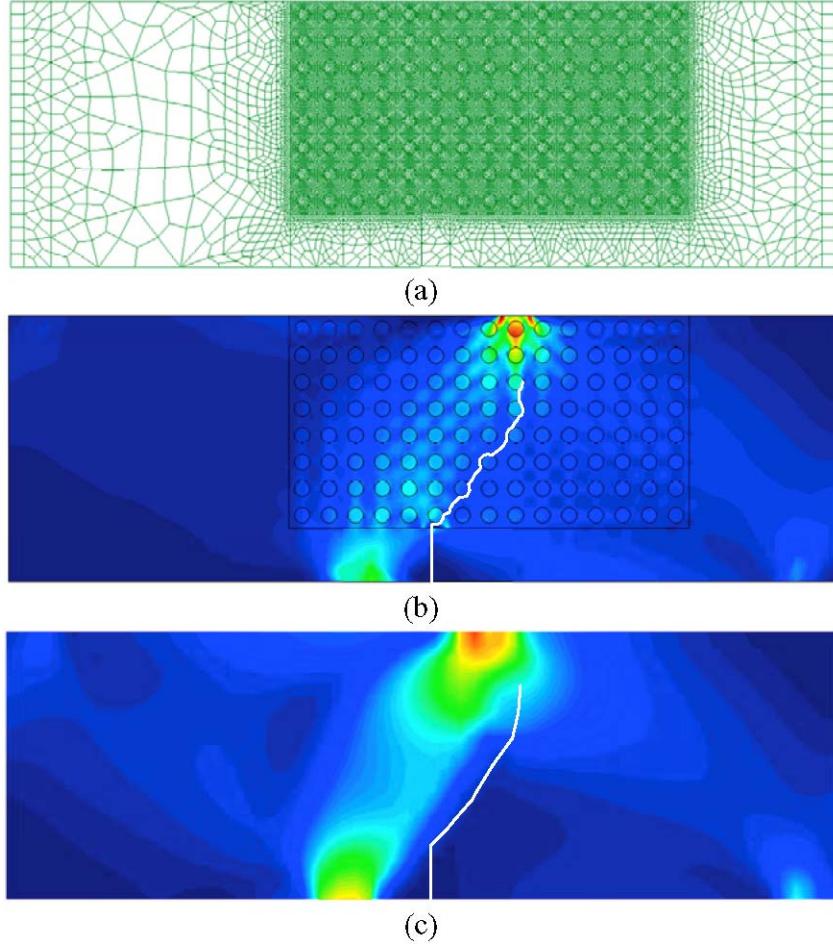
The evaluation of a multiscale method for failure poses some particular challenges. Comparison with experimental results is usually inconclusive, since the material constants for failure are not readily available. We were not able to find experiments that provide both subscale properties and a macroscale response. Therefore, we have chosen to use comparison of the multiscale results with direct numerical simulation (DNS) to evaluate the method. We show one example here: a four-point bending problem of a composite beam.

The problem is shown in Figure 1. The fibers are oriented normal to the plane of the beam. The beam is initially notched at the center on the bottom surface as shown. Figure 1 also shows the unit cells for the multiscale model. Each unit cell is represented by a finite element in the coarse scale model.



**Figure 1. Initial setup for failure of composite beam due to four-point bending.**

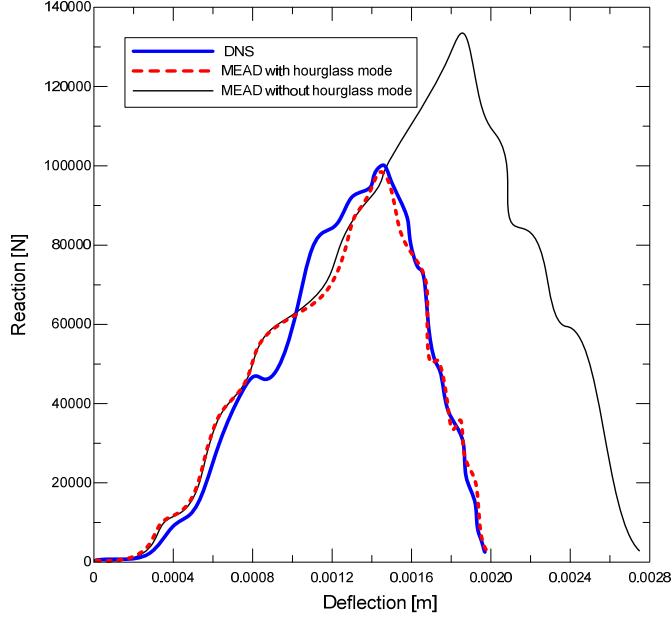
Figure 2(a) shows the DNS model, which represents the detailed structure of the composite. The crack path in the DNS model is shown in Figure 2(b). Note that the crack path for the DNS is quite jagged, since it bypasses many of the fibers. The coarse-grained solution is shown in Figure 2(c). Here the crack path is much smoother, because the subscale structure in the unit cells is not apparent to the coarse scale computation. However, the overall crack path is quite similar.



**Figure 2. Four-point bending beam problem:** (a) finite element discretization for the DNS, (b) the plots of effective stress contour for the DNS, and (c) the plots of effective stress contour for the coarse-grained MAD method.

The adequacy of the coarse scale computation by our method can be judged by the force-deflection curve shown in Figure 3. We first compare the MAD result with the hourglass mode (which is a recent improvement in the MAD method that accounts for hourgassing in the unit cell, see [1]). In that case, the agreement with the DNS solution is exceptionally good: although there are some deviations in the time history that are as large as 15%, the peak load is reproduced very well. The older method, which does not account for the hourglass deformations, agrees better in the early part of the response, but the force overshoots the DNS force significantly, which indicates that without the hourglass deformation modes the method is too stiff.

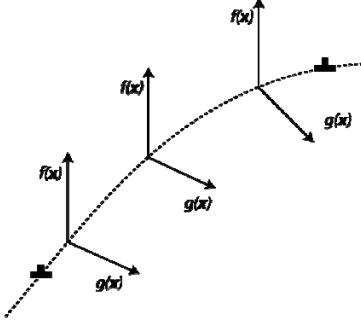
As can be seen, the multiscale method reproduces the fine scale result quite accurately. It does so with a speedup of approximately 30. This is the major benefit of multiscale methods, for without such speedups, larger problems are beyond the reach of even the largest computers.



**Figure 3. Comparison of load-deflection curves between the DNS and the MAD for the four-point bending beam problem.**

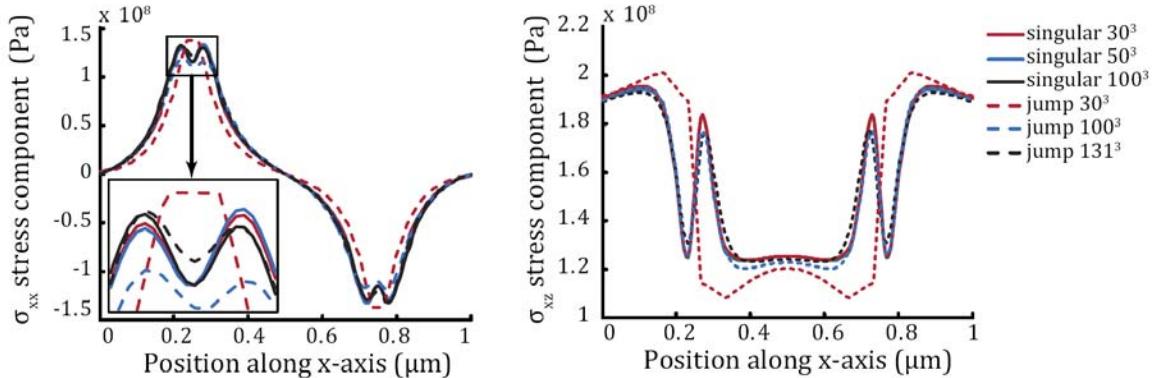
The new method for modeling dislocations is based on introducing discontinuities into the displacement field in the spirit of Volterra's concept of dislocations and the extended finite element method (XFEM) framework. The displacement field surrounding a network of dislocations in a material is represented in a finite element model by the combination of standard piecewise continuous polynomial basis functions and discontinuous enrichment functions. The enrichment functions are nonzero only in elements which have been intersected by the slip plane, and since the relative slip across the glide plane is fixed to a translation vector of the lattice, the enrichment adds no additional degrees of freedom to the discretized finite element system of equations but instead can be treated as an additional set of nodal forces. The advantage of this approach is that it can be used with complex geometries, anisotropic and non-uniform materials, and nonlinear materials [2].

A key feature of this method is the use of level set functions to describe the location of slip surfaces and dislocation lines, and the enrichment functions that inject the discontinuity across the glide plane to the solution. Each dislocation is defined by two scalar fields; the first,  $f(\mathbf{x})$ , is a signed distance function to the slip surface, and the second,  $g(\mathbf{x})$ , gives the signed distance to the dislocation line from the projection of every material point to the slip surface. Figure 4 shows how, for a curved dislocation line, the level set functions  $f$  and  $g$  vary and make up a local coordinate system around the dislocation core.



**Figure 4. Illustration of the local coordinate system defined about the core of a dislocation by the level set functions  $f(x)$  and  $g(x)$ .**

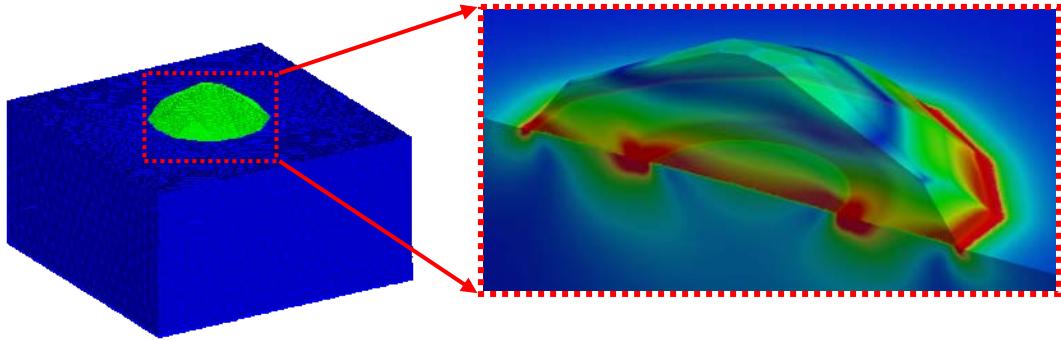
The second major component of this new method for dislocations is the construction of the enrichment functions. The simplest possibility is a constant jump across the glide surface following the Volterra construction. In addition to its simplicity, since the function is constant everywhere except for the discontinuity, there are no enrichment strains to be integrated. This is especially helpful when the dislocation line is curved because it eliminates the enrichment strain caused by the rotation of the local level set coordinate system. As shown in Oswald et al. [3] a more sophisticated option for enrichment is to take the infinite domain solutions to dislocations near the core using the local coordinate system defined by the level set functions. The analytical solutions can dramatically improve the accuracy of the computation, as shown in Figure 5 where a 27,000 element solution with singular enrichments has comparable accuracy to a two-million element solution with the jump enrichment. Both of the solutions employed a uniform mesh, so with an adaptively generated mesh the number of degrees of freedom for the jump enrichment could be significantly reduced.



**Figure 5. Comparison of  $\sigma_{xx}$  stress values on a line parallel to the x-axis passing above a circular dislocation loop lying in the x-y plane of an isotropic material for a constant jump enrichment and singular enrichments formed from the solutions of infinite-length straight dislocations.**

As an illustration of the application of this approach, consider the silicon-germanium quantum dot shown in Figure 6. This problem features several of the difficulties faced by current dislocation modeling methods. The quantum dot geometry considered here is composed of 36 facets representing 9 unique energetically favorable crystalline surfaces.

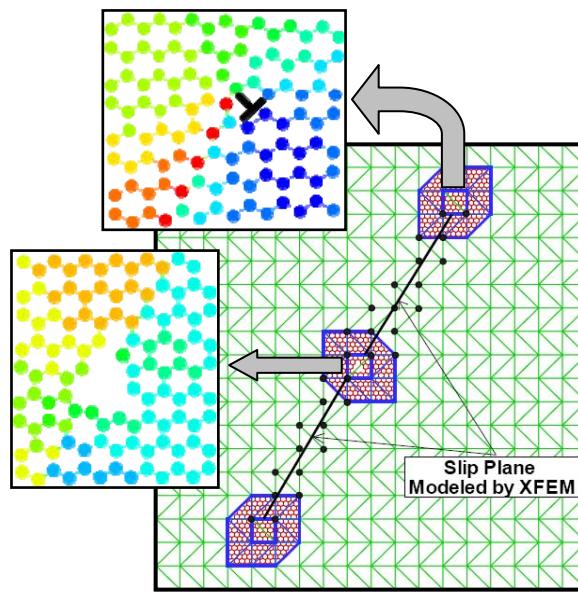
Both the quantum dot and the silicon substrate are single crystals, and therefore exhibit considerable anisotropic effects. Additionally, as reported by Malachias et al. [4] the Ge concentration varies from nearly pure germanium at the top of the quantum dot to a silicon rich core at the base. As a result, not only is there a material interface to the substrate at the base, but the elastic properties vary spatially throughout the quantum dot. Previous elastic analyses of dislocations in these structures have required the assumption of uniform isotropic material properties, but the XFEM method can treat these issues without complication.



**Figure 6.** Finite element model of a dislocation loop at the interface of a SiGe quantum dot deposited on a (001) Si surface (left), and the resulting magnitude of the stress generated by the lattice mismatch between SiGe and Si, and distortions in the lattice caused by the dislocation loop.

Another way that this dislocation method can be extended is by modeling the core structure of the dislocation by an atomistic method such as molecular statics or molecular dynamics. The modifications needed to achieve this are a suitable physical model for the interactions between atoms, a nonlinear minimization solver for molecular statics or a time integrator for molecular dynamics, and a coupling method to the continuum description of the material. To demonstrate this extension, a dislocation dipole ejected by a vacancy was modeled in a graphene sheet, where the carbon-carbon interaction energies are approximated by the Tersoff-Brenner potential. A modified version of the bridging domain method (BDM) enforces compatibility between the continuum and atomistic regions. The modification to the BDM allows the discontinuity to intersect the coupling domain such that it perfectly matches the discontinuity of atomic displacements along the slipped edges of the graphene. Figure 7 shows the computed displacement fields for the dislocation dipole and vacancy, and the XFEM enriched elements encompass the glide plane in the continuum.

This new method for dislocations makes possible the modeling of dislocations in very complex geometries and arbitrary material, including both anisotropy and nonlinearities. Furthermore, it is ideally suited for combined atomistic, continuum solutions, so it can efficiently solve large scale problems where first principles models are used for the core. This will avoid the need for phenomenological rules for the motion of the dislocations.



**Figure 7. Modeling of a dislocation ejected by a vacancy in graphene sheet by the extended finite element method coupled to a molecular mechanics simulation in the defect regions.**

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